SM4 Analyzer

Concise Introduction -- Version 4.4

A quick tour of what the program can do

Created by Dr. Larry Pai @CCMS/NTU

■ *This document is a short, non-illustrated overview -- a compact paragraph per feature -- meant to introduce what SM4 Analyzer can do, not to teach step-by-step operation. For full walkthroughs, screenshots, and appendices see the companion "sm4_analyzer_manual_full_v44.pdf" / "sm4_analyzer_manual_simple_v44.pdf". The strain-mapping physics/algorithms are covered separately in "sm4_strain_analysis_manual.pdf". A figure appendix can be prepared separately and merged with this document later (see the header comment in manual_v44_concise.py).*

Capability	Summary
Data formats	RHK SM4, Nanonis (.sxm/.3ds), Omicron SCALA/Matrix (.mtrx), Createc, PSIA/Park (.tiff), Gwyddion (.gwy, read+write), Igor ARPES cubes, LabVIEW Raman/PL-Pai (.lvm/.bin), graphic images
Spectroscopy	I-V / dI/dV / Z-V curves, CITS grid spectroscopy (with a dedicated Curve Window), ARPES 3D cubes with E-vs-k dispersion cuts, Line-STS spectral maps, Raman/PL peak fitting
Image processing	Plane/slope and background correction, CLAHE, destriping, terrace-level correction, relief shading, LUT/colour editing, drift correction
Quantitative tools	Multi-image formula tool, profiles, autocorrelation (ACF/HHCF/PSDF) with roughness statistics, particle detection, lattice-aware bond-length/angle statistics, strain mapping, Moire-pattern simulation, image merging
3D & visualization	GPU-accelerated 3D topography and ARPES-cube rendering
Output	Multi-page annotated PDF reports with compression, drawing/annotation tools, save/load of annotation "profiles"
Platform	Windows 10/11 (64-bit) and macOS, Python 3.9+

Getting Data In

2 Main Window

The launch point and control hub for the whole program: a file list plus buttons for every major window and tool (Thumbnail preview, PDF output, Cut & Paste, PDF compression, and more), arranged in labeled sections top to bottom. On smaller monitors a vertical scrollbar appears automatically so every section stays reachable.

3 File Importance Ranking

Every file can carry a 0-5 star rating and a free-text comment, entered directly in the main-window file list, used for sorting and for deciding what gets included in PDF reports. Ratings and comments save automatically to an importance.json file alongside the data.

4 Loading Files

Opens image, spectra, FFT, or 3D windows directly from a file, with duplicate and multipass-acquisition handling built in. Format is auto-detected from the file extension/folder contents, so RHK, Nanonis, Omicron, Createc, PSIA/Park, Gwyddion, ARPES-cube, and Raman/PL-Pai data are all opened the same way.

5 Thumbnail Window

A paginated grid of preview thumbnails, for all supported formats, with per-channel "jump" navigation and a two-level cache for fast browsing of large data sets. The grid auto-fits its column count to the window width, and a slider-driven derivative/contrast control defers its expensive recompute until the slider is released rather than on every drag step, to keep large directories responsive.

Core Image Analysis

6 Image Window

The primary analysis window: image display, processing, measurement, and export controls arranged in toolbar rows above and beside the plotted data -- background correction, rotation, unit-cell lattice entry, line profiles, and buttons out to FFT, 3D, Histogram, and Measure.

When the source file carries a calibrated "Temperature" status channel, the window title shows a T= reading alongside the usual bias/current fields; a scan that ran bottom-to-top is auto-mirrored back to normal orientation on load, flagged with a "(Y reverse)" tag in the title.

7 FFT Window

2D Fourier transform of the active image (or its current zoomed region), updating automatically as the parent Image window's zoom changes and always computed from native-resolution data. Includes Bragg-peak circle fitting for reciprocal-lattice vector extraction -- which then seeds the lattice-aware particle/strain-analysis tools in Section 25 -- and inverse-FFT (filtered image) output.

8 Shading / Color (LUT) Popup

Shared by the Image and FFT windows: pseudo-3D relief shading plus a colour/LUT transfer-function editor, including density-weighted piecewise colour mapping. One instance exists per parent window and keeps its settings when closed and reopened.

Spectroscopy & Mapping

9 CITS Viewer

Interactive spatial map plus selection tools for CITS (Current Imaging Tunneling Spectroscopy) grid data -- a full I(V)/dI(V) spectrum at every pixel of a scan grid -- read from RHK .sm4, Nanonis .3ds, or Omicron Matrix (via manual channel attachment). Point, rectangle, and drag-path selections can be accumulated as numbered colour groups with optional averaging; a CITS/Img switch swaps the map to the file's own topography channel for direct correlation, and selections can be pushed out to every open Image window from the same measurement session.

9a CITS Curve Window

Opens automatically on the first pixel selection in the CITS Viewer and updates in place: peak marking, group-by-group navigation, and export as PNG or CSV. A curve from a single-point selection on an ARPES-cube CITS map is labelled with its (k_x, k_y) momentum coordinates.

9b ARPES 3D Explorer

A purpose-built window for exploring energy-vs-momentum dispersion in an Igor ARPES 3-D cube: besides the usual constant-energy k_x/k_y map, the user picks an arbitrary line through k-space to view the energy-vs-distance-along-line (band-map/dispersion) cut, with smoothing, edge/high-pass filtering, and a Fermi-level (E_f) energy-axis shift.

10 Spectra Window

Displays and overlays I-V, dI/dV, and Z-V curves (or an oscilloscope trace), opening automatically when a file contains spectroscopy data; the mean of overlaid curves is drawn as a thicker line in the type's canonical colour. A companion Spectra Fit window fits peaks/curves (e.g. Gaussian/Lorentzian line shapes) directly against the displayed data.

11 ProcLineSTS -- Line STS Analysis Window

Processes and plots a full 2-D spectral dataset acquired along a line on the sample, together with the simultaneously recorded topography strip when available -- all processing and visualisation are non-destructive. Includes Transfer-to-annotation, font-size, and Star-PDF controls, plus its own in-app help.

Quantitative Tools

12 MeasureWindow

Opens via the Measure button in the Image window. Combines up to four open images (A/B/C/D -- any Image window, or the Autocorrelation window) through a numpy formula into a single Result image, which can then be measured, profiled, and exported; also hosts forward/backward drift-correction point pairs.

13 Autocorrelation Window (ACF / HHCF / PSDF)

Opens via the Correlation button in MeasureWindow and operates on its Result array (which can be picked back into MeasureWindow as a source). Computes autocorrelation, height-height correlation, and power-spectral-density functions via the FFT-based Wiener-Khinchin theorem, with a companion roughness-statistics readout for periodicity/roughness analysis and NaN border pixels (e.g. from drift correction) safely handled.

14 Histogram Window

Pixel-value distribution of the displayed (processed) image, with adjustable marker lines, cumulative-%/interval-% readouts, auto-scaling Y axis, and CSV export.

15 3D Rendering Window

GPU-accelerated (PyVista/VTK) 3D relief view of topography or ARPES data, opened via the Show 3D checkbox in the Image window, with live camera control. Requires pyvista, pyvistaqt, and PyQt5 to be installed.

Output, Annotation & Collaboration

16 PDF Output System

Assembles figures from open windows into a multi-page, 300-DPI annotated PDF report -- each "Add to PDF" action appends one or more pages -- with a built-in viewer and title annotation.

17 Transfer / Copied-Image Window (Cut & Paste)

Brings an external image (or text) into the program, or a flattened snapshot of an analysis window, onto a dedicated canvas for annotation: 16 drawing tools (lines, shapes, arrows, text, etc.) with click-to-select/deselect, Shift+click-and-drag to move any existing object, full undo/redo (Ctrl+Z / Ctrl+Y) covering both additions and moves, and Save/Load "profile" buttons that store the entire set of overlaid objects -- colour, width, and position -- to a JSON file for reuse across images.

18 PDF Compression

Reduces the saved PDF's file size by re-encoding all images as JPEG at a selectable quality level.

19 Window Layout Persistence

Remembers window positions and control settings per data channel (Z / I / dI/dV) between sessions, in sm4_analyzer_settings.json, written atomically to prevent corruption on crash or power loss.

20 Export Dialog

Central export point for images and colour maps, including the density-weighted colour mapping from the Shading/Color popup; also lists all open windows for minimize/restore management, independent of the PDF system.

Specialized & Advanced

23 Raman/PL-Pai Data Format & Curve Fitting

Reads a LabVIEW-produced Raman/PL-Pai data format in two flavours -- 1-D spectroscopy curves (.lvm) and 2-D Raman/PL maps (.bin) -- selected explicitly in the Data format dropdown or picked up by auto-detect, and fits peaks (e.g. Lorentzian/Gaussian) directly in-app.

25 Extra Analysis -- Particle, Strain, Moire & Merge

The **Extra analysis** ■ dropdown, directly above the Measure button in every Image window, is a general framework for additional per-image analysis tools -- each entry opens its own dedicated child window, seeded with the calling Image window's data. Four related modules are available: Particle/Strain Analysis, Bond Length & Angle Statistics, Strain Mapping, and Moire Analysis, plus a separate Merge Images tool -- all covered below.

25.1 Particle / Strain Analysis

Automatic detection and measurement of discrete features (particles, islands, pits, adsorbates, or individual lattice sites) in the parent Image window's currently-displayed data, via two independent detection pipelines: **Global threshold** (a conventional threshold + connected-component pipeline, with Bright/Dark, smoothing, minimum size, and manual or Auto-Otsu threshold controls) and **Lattice-aware** (predicts every lattice site from an existing FFT unit-cell fit and snaps each prediction onto the nearest real intensity peak, then reports found/missing counts).

Lattice-aware mode supports manual correction (click to add a missed site, Shift-drag to erase spurious ones, with undo and a one-click reset of manual edits) and an optional Gaussian sub-pixel center-refinement pass. Detected markers feed a live nearest-neighbor (NN) distance histogram, colour-banded by bond length, with a drag-to-select range that highlights the corresponding bonds directly on the image -- and every result exports to CSV, including the pixel centroid needed to reload a saved marker set without redoing detection.

25.1b Bond Length & Angle Statistics

A companion window, opened from Lattice-aware mode, that classifies the current NN-bond set by orientation as well as length -- sorting each bond into the nearest of several evenly-spaced orientation groups (or an "other" bucket) measured against a reference direction the user can set by dragging a line on the bond diagram, not just the image's horizontal axis. Length and orientation histograms, a colour-coded bond diagram, and a per-group statistics table (using a proper circular mean/std for angles) are produced, with CSV export of both the raw bond list and the histograms.

A "Set C" panel picks, per orientation group, either the group's own measured average bond length/angle (**relative strain**) or an independently typed-in target value such as a known bulk lattice constant (**absolute strain**) -- checking exactly two groups and clicking **Show strain maps** turns those two lengths/angles into a 2-D lattice basis and opens the Strain Mapping window below.

25.1c Strain Mapping

Every measured lattice marker is indexed, via a breadth-first walk along the real NN-bond graph starting from the centroid marker, against the 2-D lattice basis chosen in Bond Length & Angle Statistics -- so each marker's actual position can be compared with where it would sit in a perfectly unstrained lattice. The main map plots measured ("P") and reference ("S") lattices together with connector lines, so a misindexed marker is visible by eye, and exports the full measured/reference/displacement table to CSV.

A dropdown of 5 additional OVITO-style scalar maps -- each an interpolated, colour field over the marker cloud with its own colormap picker and physical scale bar -- gives a second, finer-grained view of the same strain data:

Scalar map	What it shows
Displacement magnitude |u|	Distance between each marker's measured and reference position; can switch to a signed, direction-projected component.
Shear strain	Rotation-invariant local shape distortion (zero for pure expansion/compression).
Biaxial strain	Mean in-plane normal strain -- the standard thin-film/epitaxy lattice-mismatch quantity.
Uniaxial strain (ε1 / ε2)	Strain along the two principal axes -- reveals whether local deformation is more uniaxial or biaxial.
Non-affine D^2min	Defect indicator: deviation from the best-fit locally-affine transform, spiking at dislocation cores and grain boundaries.

■ *The scientific rationale for absolute vs. relative strain, and the physics/algorithm behind every map above, is covered separately in the companion Strain Analysis Manual (sm4_strain_analysis_manual.pdf).*

25.2 Moire Analysis

A pure lattice-simulation window (it does not use the parent image's pixel data) that models the Moire superstructure from overlaying a substrate lattice (a1, a2, angle) and an overlayer lattice (b1, b2, angle) at an adjustable relative twist, shown side by side as a geometric dot overlay and a hardball (filled-disc) model with an alpha-blended Moire beat pattern. The calculated Moire period λ and Moire base vectors are printed beneath each panel.

Supports a registry-based constraint linking the overlayer's b2 length and angle, multi-atom basis loading per lattice (from a text file of fractional coordinates), an optional "Moire corrugation" proxy that grows overlayer spheres near registry with the substrate, and full persistence of every control across window reopens.

25.3 Merge Images

Composites two images (A and B) into a third, Merged, canvas by repeatedly drawing a region on A or B and pasting it -- rescaled to Merged's own nm/pixel, and optionally rotated -- at a chosen position; every step is direct mouse manipulation on the three panels, with no separate "arm" step. Selection boxes can be rotated, span the full image height/width, and be nudged by keyboard; pasted patches remain fully editable (draggable/rotatable, deletable) and Merged's pixels recompute live from the base image plus every patch's current placement.

Optional colour-coded alignment-marker pairs help line up a pasted patch with a specific target location on Merged. The finished composite opens as a brand-new, fully-interactive Image window carrying over the full file metadata of whichever source (A or B) was chosen as the Merged base. This feature is designed and preliminarily tested on RHK .sm4 data; other formats are not specifically verified.

Quick Keyboard Reference

Shortcut	Where	Effect
Ctrl+Z / Ctrl+Y	Transfer / Copied-Image window	Undo / redo drawing additions and moves
Shift+Left-click, then drag	Transfer / Copied-Image window	Select an existing object near the cursor and move it
Click a drawing tool	Transfer / Copied-Image window	Select it; click again to deselect (no tool active)
F1 or "?" button	Most windows	Open that window's in-app help
→ ← ↑ ↓	Image window line profile	Nudge the profile line
R	3D Rendering window	Reset the camera to its default view
Left-click / Shift+left-click	Particle/Strain, Merge Images windows	Add a lattice marker; place a second-lattice point or alignment marker
Left-drag on histogram	Bond Length & Angle Statistics window	Select a length/angle range for the stats readout

■ *This is a subset -- see Section 22 of the full manual for the complete keyboard-shortcut table.*